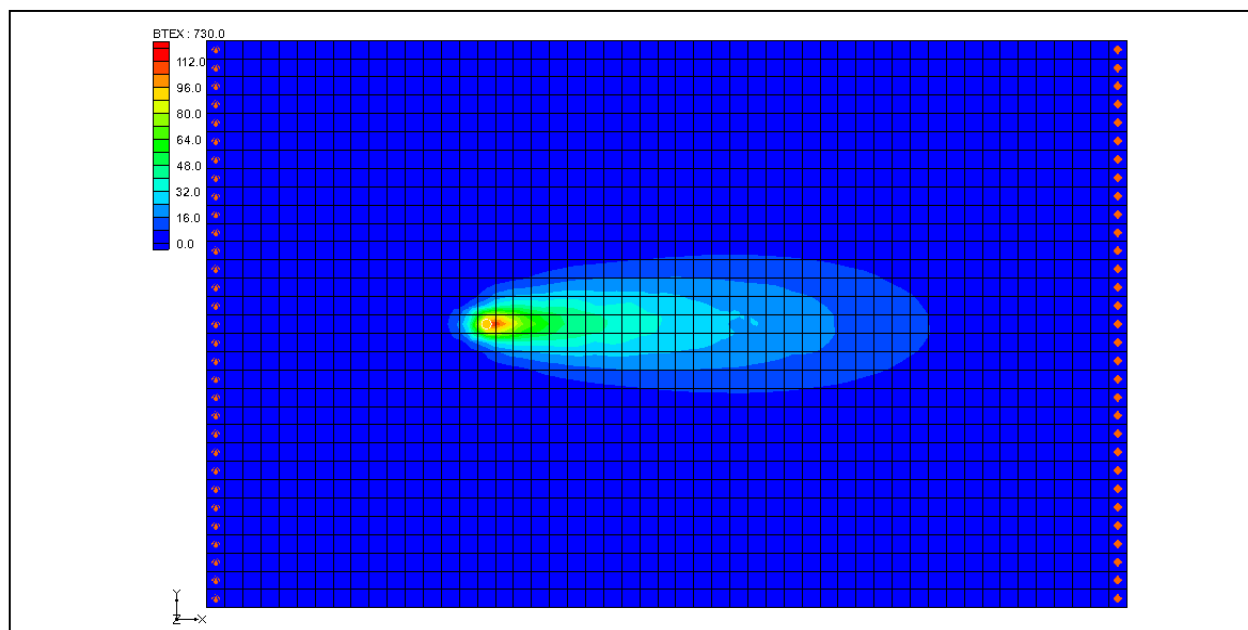*GMS 9.2 Tutorial*
RT3D – Instantaneous Aerobic Degradation

Objectives

Simulate the reaction for instantaneous aerobic degradation of hydrocarbons using a pre-defined user reaction package.

Prerequisite Tutorials	Required Components	Time
• None	• Grid • MODFLOW • RT3D	• 30-60 minutes

1 Contents

2 Introduction

This tutorial illustrates the steps involved in performing a reactive transport simulation using the RT3D model. Several types of contaminant reactions can be simulated with RT3D by using a pre-defined or user-defined reaction package. The reaction simulated in this tutorial is instantaneous aerobic degradation of hydrocarbons using a pre-defined user reaction package.

2.1 Outline

This is what you will do:

1. Create a 3D grid.

2. Define MODFLOW inputs and boundary conditions.

3. Run MODFLOW.

4. Define the transport model.

5. Run RT3D.

6. View a film loop animation.

3   Description of Problem

The problem we will be solving in this tutorial is shown in Figure 1. The site is a 510 m x 310 m section of a confined aquifer with a flow gradient from left to right. An underground storage tank is leaking fuel hydrocarbon contaminants at 2 m^3/day at the location shown. Concentration of the hydrocarbons is 1000 mg/L and the spill may be assumed to be devoid of oxygen. Details of the aquifer hydrology and geometry are given below. Initial levels of hydrocarbon and oxygen in the aquifer are 0.0 and 9.0 mg/L, respectively. We will simulate a continuous spill event and compute the resulting hydrocarbon and oxygen contours after one year using instantaneous degradation kinetics.

The first part of the problem will be to compute a flow model of the site using MODFLOW. Using the flow field computed by MODFLOW, a reactive transport model will then be defined using RT3D.
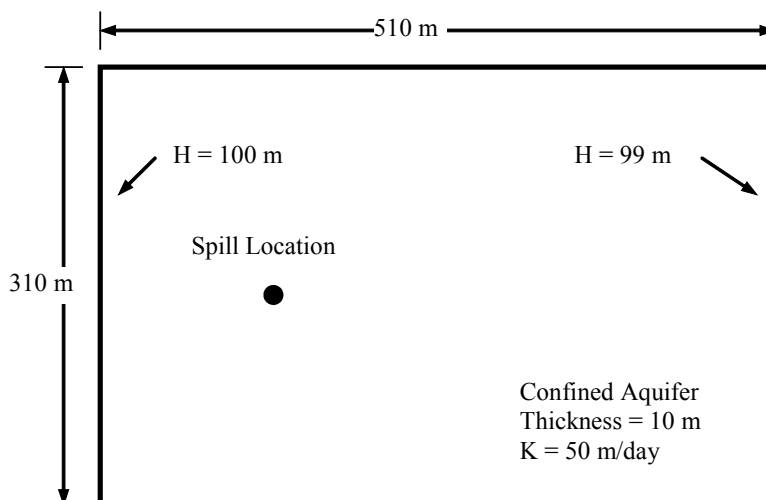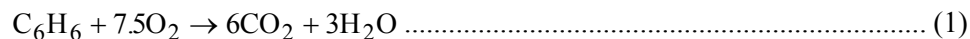

Figure 1.   Sample problem to be modeled with RT3D.

4   Description of Reaction

The reaction model we will be using simulates the instantaneous degradation of fuel hydrocarbons under aerobic conditions based on the following reaction (benzene basis):

$$C_6H_6 + 7.5O_2 \rightarrow 6CO_2 + 3H_2O \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (1)$$

Therefore, the mass ratio of benzene to oxygen, F, is 3.08 (i.e. 3.08 g of oxygen to 1 g of benzene). The instantaneous removal of either contaminant (H) or oxygen (O) is dictated by the following algorithm, where t refers to a particular time step:

$$H(t+1) = H(t) - O(t)/F \text{ and } O(t+1) = 0, \text{ when } H(t) > O(t)/F \dots\dots\dots\dots (2)$$

$$O(t+1) = O(t) - H(t) \bullet F \text{ and } H(t+1) = 0, \text{ when } O(t) > H(t) \bullet F \dots\dots\dots\dots (3)$$

Given this algorithm, either hydrocarbon or oxygen concentration in a given grid cell will be reduced to zero at each time step, depending on which component is stoichiometrically limiting in the prior time step.

5   Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *New* command from the *File* menu to ensure the program settings are restored to the default state.

6   Building the MODFLOW Model

The first part of the simulation is to build a MODFLOW flow model. In this case, a steady state flow model will be used with the transport simulation.

6.1   Conceptual Model Approach vs. Grid Approach

In many cases, the most efficient way to create a MODFLOW simulation is to build a conceptual model of the site using the feature objects in the *Map* module. However, since this problem is a simple rectangular model, we will use the grid approach and edit values directly on the cells.

6.2   Units

First, we will define the units.

1. Select the *Edit | Units* command.

2. For the *Length* unit, click the "…" button and change the vertical and horizontal units to **meters**.

3. For the *Time* unit, select **d**.

4. For the *Mass* unit, select **mg**.

5. For the *Force* unit, select **N**.

6. For the *Concentration* unit, select **mg/l**.

7. Select the *OK* button.

6.3   Creating the Grid

The first step in defining the MODFLOW simulation is to create a single layer grid.

1. In the *Project Explorer* right-click on the empty space and then, from the pop-up menu, select the *New | 3D Grid* command.

2. In the *X dimension* section, enter **510** for the *length* and **51** for the number of cells.

3. In the *Y dimension* section, enter **310** for the *length* and **31** for the number of cells.

4. In the *Z dimension* section, enter **1** for the number of cells (the length in Z does not matter).

5. Select the *OK* button.

At this point, you should see a grid appear.

6.4   Initializing the Model

Now we will initialize the MODFLOW data.

1. In the *Project Explorer* right-click on *grid* ⊞ and then, from the pop-up menu, select the *New MODFLOW* command.

6.5   The Global Package

The next step is to define the data in the MODFLOW Global Package.

Starting Head

First, we will define an initial head of 100 m everywhere in the grid.

1. Make sure the *starting heads equal grid top elevation* toggle is off.

2. Select the *Starting Heads* button.

3. Select the *Constant → Grid* button.

4. Enter a value of **100**.

5. Select the *OK* button.

6. Select the *OK* button to exit the *Starting Heads* dialog.

For the layer elevations, we will enter a value of 10.0 m for the top elevation. The bottom elevation is at zero; the existing grid already has these values, so we don't need to enter these values.

We need to change some values in the IBOUND array to designate the constant head boundaries. However, we will do this later by selecting the cells and using the *Cell Properties* command. Thus, we are finished with this dialog.

7. Select the *OK* button to exit the *Global Package* dialog.

6.6   The LPF Package

Next, we will define the data in the LPF package.

1. In the *Project Explorer* expand the *MODFLOW* item .

2. Right-click on the *LPF* package and select *Properties…*

3. Under *Layer type*, select the *Confined* option.

We will enter a horizontal hydraulic conductivity value of 50 m/day.

4. Select the *Horizontal Hydraulic Conductivity* button.

5. Select the *Constant → Grid* button.

6. Enter a value of **50**.

7. Select the *OK* button.

8. Select the *OK* button to exit the *Horizontal Hydraulic Conductivity* dialog.

The rest of the default options in the package should be sufficient.

9. Select the *OK* button to exit the *LPF Package* dialog.

6.7   Defining the Spill Well

The spill will be simulated by defining an injection well at the location of the spill with a small injection rate. During the transport simulation, a concentration will be assigned to the well. To define the well:

1. Select the *Select Cell* tool

2. While watching the I, J, K fields in the status bar, locate and right-click on the cell at I=16, J=16, K=1. Select the *Sources/Sinks…* command from the pop-up menu

3. Select the *Wells* item in the list box.

4. Select the *Add BC* button.

5. Enter a value of **2.0** for the *Q (flow)*.

6. Select the *OK* button to exit the *Sources/Sinks…*dialog.

6.8   Assigning the Head BC

The final step before running MODFLOW is to assign the constant head boundary conditions (BC) on the left and right sides of the model. First, we will assign the head BC on the left side.

1. Select the *Select J* tool

2. Right-click on any of the cells in the leftmost column in the grid, and select the *Properties…* command from the pop-up menu.

3. In the *IBOUND* row, switch the option to **Specified Head** in the pull-down list and leave the *Starting Head* value at **100.0**.

4. Select the *OK* button.

Next, we will assign the head BC on the right side.

5. Right-click on any of the cells in the rightmost column in the grid, and select the *Properties…* command from the pop-up menu.

6. In the *IBOUND* row, switch the option to **Specified Head** in the pull-down list and enter **99** for the *Starting Head* value.

7. Select the *OK* button.

6.9   Running MODFLOW

At this point, we are ready to save the model and run MODFLOW.

1. Select the *File | Save As* command.

2. In the *Save As* dialog, locate and open the directory entitled *Tutorials\rt3d\btexins1*.

3. Enter **flowmod** for the name of the simulation.

4. Select the *Save* button.

To run MODFLOW:

5. Select the *MODFLOW | Run MODFLOW* command.

6. When the simulation is finished, close the window.

GMS reads in the solution automatically. You should see a series of contours indicating a flow from left to right.

7   Building the Transport Model

Now that the flow model is established, the next step is to perform the RT3D simulation. For this part of the simulation, we will select the reaction, define the reaction data, define the supplemental layer data needed by RT3D, and assign concentrations to the well.

7.1   Initializing the Model

The first step is to initialize the RT3D data.

7. Right click on the ▦ *grid* item in the *Project Explorer* and select the *New MT3D...* command.

7.2   The Basic Transport Package

Now, we will enter the data for the Basic Transport Package. First, we will select RT3D as the transport model and select the appropriate packages.

1. In the *Model* section, select the *RT3D* option.

2. Select the *Packages* button.

3. Select the following packages:

    *   *Advection package*

    *   *Dispersion package*

    *   *Source/Sink mixing package*

    *   *Chemical reaction package*

4. Under RT3D reactions, select the **Inst. Aerobic Deg. of BTEX** option.

5. Select the *OK* button to exit the Packages dialog.

Starting Concentrations

Note that in the Layer data section of the dialog, the species associated with the reaction we are modeling are listed by name. The next step is to define the starting concentration

for each of these species. By default all of the starting concentrations are zero. This is the correct concentration for BTEX. For oxygen, we will define an ambient concentration of 9.0 mg/L.

1. Select the *Oxygen* species in the *Species* list.

2. Enter a value of **9.0** for the starting concentration.

Porosity

Next, we will define the porosity. The aquifer is a uniform horizontal aquifer with a top elevation of 10 m, a thickness of 10 m, and a porosity of 0.3. Since 0.3 is the default porosity assigned by GMS, no changes need to be made.

Stress Periods

Next, we will define the stress periods. Since the injection rate and the boundary conditions do not change, we will use a single stress period with a length of 730 days (two years).

1. Select the *Stress Periods* button.

Since there is already one stress period by default, we will simply change the length of the stress period

2. Enter a value of **730** for the *Length*.

3. Enter a value of **10** for the *Number of time steps*.

4. Select the *OK* button to exit the *Stress Periods* dialog.

Output Options

Finally, we will define the output options. One binary solution file is created by RT3D for each of the species. By default, RT3D saves a solution at each transport step for each species. Since this results in large files containing more solutions than we need for the simple post-processing we intend to do, we will specify that a solution be saved every 73 days (every time step).

1. Select the *Output Control* button.

2. Select the *Print or save at specified times* option.

3. Select the *Times* button.

4. Select the *Initialize Values* button.

5. Enter **73.0** for the *Initial time step size*.

6. Enter **73.0** for the *Maximum time step size*.

7. Enter **730.0** for the *Maximum simulation time*.

8. Select the *OK* button to exit the *Initialize Time Steps* dialog

9. Select the *OK* button to exit the *Variable Time Steps* dialog.

10. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

11. Select the *OK* button to exit the *Basic Transport Package* dialog.

7.3   Assigning Concentrations to the Left Boundary

The left boundary of the model is a constant head boundary. Since the head at the left boundary is greater than the head at the right boundary, the left boundary acts as a source and water enters the model from the left. Thus, we must define the concentrations of our species at the left boundary. Otherwise, the water entering the model will have the default concentration (zero) for each of the species. This is often true for most species, but there are exceptions. For our model, the incoming fluid should have an ambient oxygen concentration of 9.0 mg/L. The oxygen concentration can be assigned one of two ways:

1. The cells at the boundary can be marked as specified concentration cells by changing the ICBUND value at the cells to –1.

2. The concentration of the incoming fluid at the boundary can be defined using the Source/Sink Mixing package.

The first method requires the fewest number of steps to set up. As long as the boundary acts as a source throughout the simulation, either of these approaches will achieve the same result. However, if the boundary acts as a sink during any part of the simulation, the second option should be used. With the second option, if the boundary switches to a sink due to changing heads in the interior of the model, the concentrations at the cells would be computed by RT3D. With the first option, the concentrations at the cells are fixed, regardless of the flow direction.

For our problem, the flow field is steady state and we know that the boundary acts as a source. Thus, we will use the first option. To mark the cells as specified concentration cells:

3. Select the *Select Cells* tool 🔲

4. Select the cells on the left boundary by dragging a box that just surrounds the cells.

5. Select the *MT3D | Cell Properties…* command.

6. Change the *ICBUND* value to **-1**.

7. Select the *OK* button.

Note that we do not need to change the starting concentration values, since the values are already assigned via the starting concentration arrays.

7.4   The Advection Package

The next step is to initialize the data for the Advection package. We will be using the MOC method.

1. Select the *RT3D | Advection Package* command.

2. In the Solution scheme section, select the **Method of characteristics (MOC)** method.

3. Select the *OK* button.

7.5   The Dispersion Package

Next, we will enter the data for the Dispersion package. The aquifer has a longitudinal dispersivity of 10.0 m and a transverse dispersivity of 3.0 m. The vertical dispersivity is assumed equal to the longitudinal dispersivity.

1. Select the *RT3D | Dispersion Package* command.

2. Select the *Longitudinal Dispersivity* button.

3. Select the *Constant* $\rightarrow$ *Grid* button.

4. Enter a value of **10.0** and select *OK*.

5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.

6. Enter a value of **0.3** for the *TRPT* value.

7. Select the *OK* button to exit the *Dispersion Package* dialog.

7.6   The Source/Sink Mixing Package

Next, we must define the concentration at the spill location. To define the source at the spill location, we need to select the well and assign a concentration.

1. Select the cell containing the injection well (spill location) by clicking anywhere in the interior of the cell.

2. Select the *RT3D | Point Sources/Sinks* command.

3. Click the *Add BC* button near the bottom of the dialog.

4. Change the *Type (ITYPE)* to **well (WEL)**.

5. In the *BTEX* column, enter a concentration of **1000** (mg/L).

6. Leave the oxygen at the default value of **0.0**.

7. Select the *OK* button to exit the dialog.

7.7   The Chemical Reactions Package

The final step is to initialize the data for the Chemical Reactions package. In this case, the default values are adequate and no changes are necessary.

7.8   Running RT3D

We are now ready to save the model and run RT3D. We will save the current project under a different name than the MODFLOW model. Because of this, we need to explicitly tell RT3D the name of the MODFLOW model.

1. Select the *RT3D | Run Options* command.

2. Select the *Single run with selected MODFLOW solution* option. Confirm that the **flowmod (MODFLOW)** solution is selected, and hit *OK*.

3. Select the *File | Save As* command.

4. In the *Save As* dialog, check to make sure the path is still set to *Tutorials\rt3d\btexins1*.

5. Enter **btexmod** for the file name.

6. Select the *Save* button.

To run RT3D:

7. Select the *RT3D | Run RT3D* command.

8. When the simulation is finished, select the *Close* button.

GMS will read in the solution automatically.

7.9   Viewing the Results

The contours you see are for BTEX at the end of the first time step (73.0 days). To view the BTEX solution at 730 days:

1. Expand the *btexmod (RT3D)* solution in the *Project Explorer*.

2.   Select the *BTEX* data set 🖼.

The *Time Step Window* should now appear below the *Project Explorer*. The *Time Step Window* is set to appear when a transient dataset is selected in the *Project Explorer*.

3.   Select the **730.0** time step in the *Time Steps Window*.

To get a better plot of the concentration contours:

4.   Select *Contour Options* 🔸 from the main toolbar.

5.   Select the **Color Fill** option for the *Contour Method*.

6.   Select the *OK* button to exit the *Contour Options* dialog.

Next, we will view the Oxygen solution at 730 days.

7.   Select the *Oxygen* data set 🖼 in the *Project Explorer*.

You may wish to use the *Project Explorer* and *Time Steps* window to view the solution at other time steps.

7.10   Viewing a Film Loop Animation

The most effective post-processing tool for transient data is a film loop animation. We will set up an animation showing the fate of the BTEX through the entire duration of the simulation.

1.   Select the *BTEX* data set 🖼 in the *Project Explorer*.

To set up the animation:

2.   Select the *Display | Animate* command.

3.   Make sure the *Data set* option is on and click *Next*.

4.   Turn on the *Display clock* option.

5.   Select the *Finish* button.

6.   After viewing the animation, select the *Stop* ■ button to stop the animation.

7.   Select the *Step* ▶| button to move the animation one frame at a time.

8.   You may wish to experiment with some of the other playback controls. When you are finished, close the window and return to GMS.

This concludes the tutorial.